Ground State Energy of the Low Density Fermi Gas

Elliott H. Lieb and Robert Seiringer

Department of Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton NJ 08544, USA

Jan Philip Solovej

Department of Mathematics, University of Copenhagen, Universitetsparken 5, DK-2100 Copenhagen, Denmark

(Dated: Dec. 21, 2004)

Recent developments in the physics of low density trapped gases make it worthwhile to verify old, well known results that, while plausible, were based on perturbation theory and assumptions about pseudopotentials. We use and extend recently developed techniques to give a rigorous derivation of the asymptotic formula for the ground state energy of a dilute gas of N fermions interacting with a short-range, positive potential of scattering length a. For spin 1/2 fermions, this is $E \sim E^0 + (\hbar^2/2m)2\pi N \rho a$, where E^0 is the energy of the non-interacting system and ρ is the density. A similar formula holds in 2D, with ρa replaced by $\rho / |\ln(\rho a^2)|$. Obviously this 2D energy is not the expectation value of a density-independent pseudopotential.

I. INTRODUCTION

The leading asymptotics for the ground state energy of a dilute gas of fermions, interacting with a positive, short range pair potential, was derived years ago by several approximate methods [1, 2, 3]. Indeed, the leading correction beyond the ideal gas formula is no different for fermions than for bosons, except for the fact that all bosons interact with each other whereas the spin-up fermions effectively interact only with the spin-down fermions and not with each other. In this sense, the formula goes back to Lenz [4] who derived the energy formula for bosons by assuming that each particle interacts with N-1 fixed particles that are well spaced from each other.

Thus, we expect that the ground state energy per unit volume, $e(\varrho_{\uparrow}, \varrho_{\downarrow})$, for N_{\uparrow} spin-up particles and N_{\downarrow} spin-down particles of mass m in a box of volume V (in the usual thermodynamic limit in which $V \to \infty$ and $\varrho_{\uparrow} = N_{\uparrow}/V$ and $\varrho_{\downarrow} = N_{\downarrow}/V$ are fixed) is, asymptotically,

$$e(\varrho_{\uparrow}, \varrho_{\downarrow}) = \frac{\hbar^2}{2m} \frac{3}{5} (6\pi^2)^{2/3} \left(\varrho_{\uparrow}^{5/3} + \varrho_{\downarrow}^{5/3} \right) + \frac{\hbar^2}{2m} 8\pi a \varrho_{\uparrow} \varrho_{\downarrow} + \text{higher order in } (\varrho_{\uparrow}, \varrho_{\downarrow}) , \qquad (1)$$

where a is the two-body (s-wave) scattering length of the pair potential v. Under the assumption that the total density $\varrho \equiv \varrho_{\uparrow} + \varrho_{\downarrow}$ is fixed, this formula indicates that at low density the absolute ground state has spin zero, i.e., $\varrho_{\uparrow} = \varrho_{\downarrow} = \varrho/2$.

The corresponding low density formula for bosons contains only one kind of density and is

$$e(\varrho) = \frac{\hbar^2}{2m} 4\pi a \varrho^2 + \text{higher order in } \varrho . \tag{2}$$

This asymptotic formula was proved rigorously in [5].

It is customary, nowadays, to regard (1) as coming from a pseudopotential $\frac{\hbar^2}{2m}8\pi a\delta(x_i-x_j)$, and that is certainly a useful shortcut to obtaining current results. But this has to be justified mathematically, and that is the purpose of

this paper. Several issues of physical interest are involved, which make it not totally obvious that the pseudopotential approach is beyond need of justification.

- The availability of a good variational function Ψ is important in theoretical physics, one that correctly displays the correlations of physical interest and whose energy $\langle \Psi | H | \Psi \rangle$ (which is necessarily an upper bound to the ground state energy) can be computed without resort to uncontrolled approximations. It should also give the correct energy to the desired accuracy. A good example is the BCS function of superconductivity. In the boson problem one would think of a Bijl-Dingle-Jastrow function $J = \prod_{i,j} g(x_i x_j)$ but it has not been possible, as far as we know, to carry out the energy calculation without making assumptions. The correlations are subtle (even if they are physically clear) and have to be treated carefully, and the required rigorous bosonic upper bound was finally found by Dyson [6] but by using a non-bosonic variational function. In the fermionic case considered here we use a function of the form $\Psi = S \cdot J$, where S is a Slater determinant. While this Ψ looks simple, the calculation of an upper bound of the required accuracy (1) occupies half of this paper, and one cannot say that this is a simple calculation.
- The source of difficulties in the boson problem is the subtlety of the correlations, which constitute the entire energy. In the fermionic case, on the other hand, we are looking for a tiny correction to a dominant free-particle kinetic energy, but this contribution, especially for hard-core potentials, does not come from a small perturbation. It is not obvious that hard core collisions do not create energy changes by perturbing the Fermi surface.
- The pseudopotential idea, while attractive, does have the drawback that it cannot be right in two dimensions (2D). The quantity $a\varrho^2$ for 3D bosons is replaced by $\varrho^2/|\ln(\varrho a^2)|$, as predicted by [7, 8] and proved in [9]. (Note: The scattering length can be defined in 2D as well as 3D. See [9].) Consequently, the pseudopotential will have to depend on ϱ . Thus, for fermions the energy to leading order in ϱa^2 ought to be

$$e(\varrho_{\uparrow}, \varrho_{\downarrow}) = \frac{\hbar^2}{2m} 2\pi \left(\varrho_{\uparrow}^2 + \varrho_{\downarrow}^2\right) + \frac{\hbar^2}{2m} \frac{8\pi}{|\ln(\varrho a^2)|} \varrho_{\uparrow} \varrho_{\downarrow} + \text{higher order in } (\varrho_{\uparrow}, \varrho_{\downarrow}) . \tag{3}$$

We will prove formula (3) as well. Fermions in two dimensional layers are physically interesting and it can be useful to have (3) proved rigorously.

• In addition to the pseudopotential approach there is also the approach of summing diagrams [10], which leads to many terms beyond the two in (1). Nevertheless, it has to be admitted that expansions, especially where hard-core potentials are concerned, may have convergence or other difficulties. Effective field theory methods have also been used successfully [11], but with similar concerns. Therefore, rigorous confirmation is much to be desired and we provide it here.

In the following we do everything in 3D until Section VI, where we explain the modifications necessary for 2D, some of which are not trivial. This is done in order to make the essential ideas as clear as possible. In a forthcoming paper [12], the natural generalization of (1) to positive temperature states will be proved.

II. MODEL AND MAIN RESULTS

In units in which $\hbar^2/2m = 1$ (which will be used henceforth), and with $\Delta = \nabla^2$, the Hamiltonian is given by

$$H = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \le i < j \le N} v(x_i - x_j), \tag{4}$$

acting on anti-symmetric functions of N space-spin variables, i.e., functions in $\bigwedge^N L^2(\Lambda; \mathbb{C}^q)$. Here $q \geq 1$ denotes the number of spin states. The particles are confined to a bounded region Λ , which we choose to be a cube of side length L and volume $V = L^3$ (or L^2 in 2D). We choose Dirichlet boundary conditions for the Laplacian, i.e., $\Psi = 0$ when any x_i is on the boundary of the cube.

Since H is spin-independent, we can specify the number of particles of each spin, N_1, N_2, \ldots, N_q with $N = \sum_j N_j$. The wave function Ψ is then a function of the N coordinates x_1, \ldots, x_N , without mention of spin at all, but with the requirement on Ψ that it be antisymmetric separately in the first N_1 variables, the second N_2 variables, etc. To avoid needless notation we will give our proofs for q = 2 but will state the main Theorems 1 and 2 for general q.

The pair potential v(x) is assumed to be positive, radial, and of finite range R_0 . It then has a finite and positive scattering length a. The scattering length can be defined as follows: if $\varphi(x)$ is the unique solution (see [9] for a full discussion) of the zero-energy scattering equation

$$-\Delta\varphi(x) + \frac{1}{2}v(x)\varphi(x) = 0 \tag{5}$$

subject to the boundary condition $\lim_{|x|\to\infty} \varphi(x) = 1$, then a is given by $a = \lim_{|x|\to\infty} |x|(1-\varphi(x))$. Note that we do not assume v to be integrable; our results also apply to the case of a hard core. Note also that for a pure hard-core interaction, the scattering length is equal to the range.

There is no need (apart from simplicity) to assume that the potentials v(x) between different groups of particles are the same, thereby allowing the Hamiltonian to be 'spin-dependent'. Thus, we could take the pair potential to be $v_{i,j}(x)$, (with $1 \le i, j \le q$) between groups i and j, with corresponding scattering lengths $a_{i,j}$. In this way, the quantity $a\varrho_i\varrho_j$ in Theorem 1 would be replaced by $a_{i,j}\varrho_i\varrho_j$. Our proof would still go through with obvious trivial changes.

Our main result concerns the ground state energy $E_0(\{N_i\}, L)$ of H, in the thermodynamic limit $L \to \infty$ with $\varrho_i = N_i/L^3$ fixed. It is well known that for systems with short range interactions the limit of the energy density, $E_0(\{N_i\}, L)/L_3$ exists and is independent of boundary conditions [13, 14].

Theorem 1. Fix $\varrho_i = N_i/L^3$ for $1 \le i \le q$ and $\varrho = \sum_i \varrho_i$, and let $E_0(\{N_i\}, L)$ denote the ground state energy of H with the appropriate antisymmetry in each of the N_i coordinate variables. Then, for small ϱ ,

$$\lim_{L \to \infty} \frac{1}{L^3} E_0(\{N_i\}, L) = \frac{3}{5} \left(6\pi^2\right)^{2/3} \sum_{i=1}^q \varrho_i^{5/3} + 8\pi a \sum_{1 \le i < j \le q} \varrho_i \,\varrho_j + a\varrho^2 \varepsilon(\varrho),\tag{6}$$

 $\mbox{\it with } -\mbox{const.} \, \left(a\varrho^{1/3}\right)^{1/13} \leq \varepsilon(\varrho) \leq +\mbox{const.} \, \left(a\varrho^{1/3}\right)^{2/9}.$

The constants in the bounds on $\varepsilon(\varrho)$ depend on the interaction potential only through the dimensionless ratio R_0/a . We could, in principle, display the explicit dependence on R_0/a . By cutting off an infinite range potential in an

appropriate way, this would allow us to extend the result (with different bounds on $\varepsilon(\varrho)$) to infinite-range potentials with finite scattering length.

The analogous theorem in 2D is the following.

Theorem 2. Fix $\varrho_i = N_i/L^2$ for $1 \le i \le q$ and $\varrho = \sum_i \varrho_i$, and let $E_0(\{N_i\}, L)$ denote the ground state energy of H with the appropriate antisymmetry in each of the N_i coordinate variables. Then, for small ϱ ,

$$\lim_{L \to \infty} \frac{1}{L^2} E_0(\{N_i\}, L) = 2\pi \sum_{i=1}^q \varrho_i^2 + \frac{8\pi}{|\ln(\varrho a^2)|} \sum_{1 \le i \le j \le q} \varrho_i \,\varrho_j + \frac{\varrho^2}{|\ln(\varrho a^2)|} \varepsilon(\varrho),\tag{7}$$

with $-\text{const.} |\ln(a^2\varrho)|^{-1/10} \le \varepsilon(\varrho) \le +\text{const.} |\ln(a^2\varrho)|^{-1} \ln|\ln(a^2\varrho)|$.

For simplicity we consider only q=2 henceforth, i.e., the spin $\frac{1}{2}$ case. The extension to general $q\geq 2$ is straightforward. We introduce the following convenient notation. For $N_1+N_2=N$, let $X=(x_1,\ldots,x_{N_1})$ and $Y=(y_1,\ldots,y_{N_2})$ stand for the collection of spin-up and spin-down particle coordinates, respectively. The Hamiltonian can then be written as

$$H = -\Delta_X - \Delta_Y + v_{XX} + v_{YY} + v_{XY},\tag{8}$$

with $\Delta_X = \nabla_X^2 = \sum_{i=1}^{N_1} \nabla_{x_i}^2$, $\Delta_Y = \nabla_Y^2 = \sum_{i=1}^{N_2} \nabla_{y_i}^2$, $v_{XX} = \sum_{i < j} v(x_i - x_j)$, and $v_{XY} = \sum_{i,j} v(x_i - y_j)$. It acts on the Hilbert space of square-integrable functions that are antisymmetric in the X and in the Y variables.

III. OUTLINE OF PROOF

Before presenting the proof of Theorems 1 and 2 in full detail, we give a short outline. We first concentrate on the three-dimensional case. The proof is split into two parts, the upper and lower bounds to the ground state energy. The upper bound, given in Section IV, uses the variational principle. The idea is to construct a trial wave function that shows the features one would expect the true ground state to have, but is at the same time sufficiently simple to make it possible to compute a good upper bound on the expectation value of the Hamiltonian. For this latter purpose we find it necessary to choose a function that confines the particles to small boxes, separated from each other to avoid interaction between different boxes. These boxes must not be chosen too small, however, to ensure that the finite size effects are negligible compared to the leading term in the interaction energy. Since this latter energy is rather small, we are forced to have a large number of particles in each of the boxes. This makes it impossible to control the norm of our trial wave function, and hence we must carefully take into account cancellations between the ratio of the expectation value of the Hamiltonian and the norm of the trial wave function.

For the lower bound to the energy, given in Section V, the first essential step is to replace the 'hard' interaction potential v(x) by a 'soft' one, W(x), at the expense of using up some positive kinetic energy. This idea goes back to Dyson [6], who computed a lower bound for the ground state energy of a hard-sphere Bose gas. Only the high-momentum part of the kinetic energy is dispensable, however, since the low-momentum part is needed to fill the Fermi sea. In Lemma 4 below we prove such a bound, using only momenta bigger than a certain cutoff. With the soft potential W(x) one can then hope to proceed with some sort of rigorous perturbation theory to obtain a lower bound to the energy. Indeed, we prove two a priori bounds, one on the one-particle density matrix of the ground state, showing that it is close to the projection onto the Fermi sea, and another one on the number of particles whose

distance to their nearest neighbor is small. These bounds can be used to show that the ground state expectation of W(x) has the anticipated value.

The necessary modifications of our proofs for the corresponding result in two dimensions, Theorem 2, are sketched in Section VI.

IV. UPPER BOUND TO THE GROUND STATE ENERGY

We start by collecting some properties of the solution to the 3D zero-energy scattering equation (5). The proofs can be found in the appendix of [9]. The solution to (5), $\varphi(x)$, is a radial function and satisfies

- $0 \le \varphi(x) \le 1$, and hence a > 0.
- $\varphi(x)$ is subharmonic on \mathbb{R}^3 (i.e., $\Delta \varphi(x) \geq 0$, see [15]), $\Delta \varphi(x)$ is a positive measure which is zero for $|x| > R_0$, and $\int_{\mathbb{R}^3} \Delta \varphi(x) \, d^3x = 4\pi a$.
- $\varphi(x) \ge 1 a/|x|$, and $\varphi(x) = 1 a/|x|$ for $|x| \ge R_0$.
- $\int_{|x| < R} (|\nabla \varphi(x)|^2 + \frac{1}{2}v|\varphi(x)|^2) d^3x = 4\pi a(1 a/R)$ for $R \ge R_0$.

These properties will be useful both for the upper bound given in this section and the lower bound given in the next.

For the upper bound, it will be convenient to localize the particles into small boxes with Dirichlet boundary conditions. The number of particles in each box will be large for small ϱ , but finite and independent of the size of the large container V. Let the side length the small boxes be ℓ . If we place these small boxes a distance R_0 from each other, then there will be no interaction between particles in different boxes. We then want to put $n = \varrho_1(\ell + R_0)^3$ spin-up particles into each box, and likewise $m = \varrho_2(\ell + R_0)^3$ spin-down particles. Since $\varrho_i(\ell + R_0)^3$ need not be an integer, however, we will choose

$$n = \varrho_1(\ell + R_0)^3 + \varepsilon_1$$
 and $m = \varrho_2(\ell + R_0)^3 + \varepsilon_2$, (9)

with $0 \le \varepsilon_1, \varepsilon_2 < 1$ chosen such that n and m are integers. We then really have too many particles, but this is legitimate for an upper bound, since the energy is certainly increasing with particle number. We thus have

$$\lim_{L \to \infty} \frac{1}{L^3} E_0(N_1, N_2, L) \le \frac{1}{(\ell + R_0)^3} E_0(n, m, \ell), \tag{10}$$

with n and m given as in (9). This bound holds for all choices of the box size ℓ .

We will now derive an upper bound on the ground state energy of n spin-up and m spin-down particles in a cubic box of side length ℓ , for general n, m and ℓ . We take as a trial state the function

$$\Psi(X,Y) = D_n(X)D_m(Y)G_n(X)G_m(Y)F(X,Y), \tag{11}$$

where $D_n(X)$ denotes the Slater determinant of the first n eigenfunctions of the Laplacian in a cubic box of side length ℓ , with Dirichlet boundary conditions. (In the case of degeneracy, any choice will do.) Moreover,

$$G_n(X) = \prod_{1 \le i < j \le n} g(x_i - x_j), \tag{12}$$

with $0 \le g(x) \le 1$, having the property that g(x) = 0 for $|x| \le s$ and g(x) = 1 for $|x| \ge 2s$, for some $s > 2R_0$ to be chosen later. We can assume that $|\nabla g(x)| \le \text{const. } s^{-1}$ for some constant independent of s. Finally,

$$F(X,Y) = \prod_{i=1}^{n} \prod_{j=1}^{m} f(x_i - y_j), \tag{13}$$

with $f(x) = \varphi(x)/(1-a/R)$ for $|x| \le R$ and 1 otherwise. Here $\varphi(x)$ denotes the solution to the zero-energy scattering equation, and we assume that $R > R_0$, which guarantees that f is a continuous function. Moreover, we assume $2R \le s$. By the variational principle,

$$E_0(n, m, \ell) \le \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$
 (14)

Since Ψ vanishes whenever two particles of the same kind are closer together than the range of the interaction, we have

$$\langle \Psi | H | \Psi \rangle = \langle \Psi | -\Delta_X | \Psi \rangle + \langle \Psi | -\Delta_Y | \Psi \rangle + \langle \Psi | v_{XY} | \Psi \rangle.$$

In evaluating the kinetic energy, we use partial integration and the fact that $D_n(X)$ is an eigenfunction of $-\Delta_X$. Let the corresponding eigenvalue (namely the sum of the lowest n eigenvalues of the Dirichlet Laplacian) be denoted by $E^{\mathcal{D}}(n,\ell)$. Then

$$\begin{split} \langle \Psi | - \Delta_X | \Psi \rangle \; &= \; E^{\mathrm{D}}(n,\ell) \langle \Psi | \Psi \rangle \\ &+ \int D_n(X)^2 |\nabla_X G_n(X) F(X,Y)|^2 D_m(Y)^2 G_m(Y)^2 \, dX \, dY. \end{split}$$

Here we denoted $dX = \prod_{i=1}^{n} d^3x_i$ and $dY = \prod_{j=1}^{m} d^3y_j$ for short. In the second term, we use the Schwarz inequality to deduce (for some $\varepsilon > 0$ to be chosen later)

$$|\nabla_X G_n(X) F(X,Y)|^2 \le (1+\varepsilon) |\nabla_X F(X,Y)|^2 G_n(X)^2$$
$$+ (1+\varepsilon^{-1}) F(X,Y)^2 |\nabla_X G_n(X)|^2.$$

Proceeding in the same way for the kinetic energy of the Y-particles, we thus get the upper bound

$$\langle \Psi | H | \Psi \rangle \le I + (1 + \varepsilon)II + (1 + \varepsilon^{-1})III,$$
 (15)

with

$$I = \left[E^{D}(n,\ell) + E^{D}(m,\ell) \right] \langle \Psi | \Psi \rangle, \tag{16}$$

$$II = \int \left[|\nabla_X F(X,Y)|^2 + |\nabla_Y F(X,Y)|^2 + v_{XY} F(X,Y)^2 \right] D_n(X)^2 D_m(Y)^2 G_n(X)^2 G_m(Y)^2 dX dY, \tag{17}$$

and

$$III = \int \left[|\nabla_X G_n(X)|^2 G_m(Y)^2 + |\nabla_Y G_m(Y)|^2 G_n(X)^2 \right] F(X, Y)^2 D_n(X)^2 D_m(Y)^2 dX dY. \tag{18}$$

The positivity of v_{XY} has been used here. We shall now bound these three terms, when divided by $\langle \Psi | \Psi \rangle$, separately.

We start with I. We may consider the sum of the n lowest Dirichlet eigenvalues as a Riemann sum for the integral

$$(\ell/\pi)^3 \int_{\substack{|p| \le k_{\rm F}, \\ p_1, p_2, p_3 \ge 0}} p^2 d^3p = \frac{3}{5} (6\pi^2)^{2/3} \frac{n^{5/3}}{\ell^2},$$

where we denote the Fermi momentum by $k_{\rm F} = (6\pi^2 n)^{1/3}/\ell$. It is then easy to see that

$$E^{\mathcal{D}}(n,\ell) \le \frac{3}{5} (6\pi^2)^{2/3} \frac{n^{5/3}}{\ell^2} \left(1 + \text{const.} \, n^{-1/3} \right),$$
 (19)

and the exponent in the error term is actually optimal. We note that this bound shows that we must not choose ℓ too small in order to have an error term that is negligible compared with $a\varrho$; more precisely, we need $n \sim \varrho_1 \ell^3 \gg (a^3 \varrho)^{-1}$. This will be fulfilled with our choice of ℓ below.

Next we derive an upper bound on II. We are going to need the following lemma.

Lemma 1. Let $D_n(X)$ denote a Slater determinant of n linearly independent functions $\phi_{\alpha}(x)$. For a given function h(x) of one variable, let $\Phi(X)$ be the function $\Phi(X) = D_n(X) \prod_{i=1}^n h(x_i)$, and let M denote the $n \times n$ matrix

$$M_{\alpha\beta} = \int \phi_{\alpha}^*(x)\phi_{\beta}(x)|h(x)|^2 d^3x. \tag{20}$$

Then

- (i) The norm of Φ is given by $\langle \Phi | \Phi \rangle = \det M$.
- (ii) For $1 \le k \le n$, the k-particle densities of Φ are given by

$$\binom{n}{k} \frac{1}{\langle \Phi | \Phi \rangle} \int |\Phi(X)|^2 d^3x_{k+1} \cdots d^3x_n = \frac{1}{k!} \prod_{i=1}^k |h(x_i)|^2 (x_1 \wedge \cdots \wedge x_k | M^{-1} \otimes \cdots \otimes M^{-1} | x_1 \wedge \cdots \wedge x_k),$$

where $|x\rangle$ denotes the n-dimensional vector with components $\phi_{\alpha}(x)$, $1 \leq \alpha \leq n$, and $|x_1 \wedge \cdots \wedge x_k\rangle$ stands for the Slater determinant $(k!)^{-1/2} \sum_{\sigma} (-1)^{\sigma} |x_{\sigma(1)}\rangle \otimes \cdots \otimes |x_{\sigma(k)}\rangle$, σ denoting permutations.

(iii) If $\Phi'_i(X) = \Phi(X)k(x_i)/h(x_i)$ for some function k(x), then

$$\sum_{i=1}^{n} \langle \Phi_i' | \Phi_i' \rangle = \left(\det M \right) \left(\operatorname{Tr} \left[K M^{-1} \right] \right), \tag{21}$$

where $\text{Tr}[\cdot]$ denotes the trace, and K is the $n \times n$ matrix

$$K_{\alpha\beta} = \int \phi_{\alpha}^*(x)\phi_{\beta}(x)|k(x)|^2 d^3x. \tag{22}$$

The proof of this lemma is a straightforward exercise that we leave to the reader. Note that without loss of generality one can set h(x) = 1 in proving the lemma. Item (iii) is an immediate consequence of items (i) and (ii), noting that the left side of (21), when divided by the norm of $\Phi(X)$, is the integral of the one-particle density of $\Phi(X)$ multiplied by $|k(x)/h(x)|^2$; we state it as a separate item for later use.

Using $G_n(X) \leq 1$, we infer from this lemma that, for any fixed Y,

$$\int G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \frac{1}{2} v_{XY} |F(X,Y)|^2 \right] dX$$

$$\leq \int D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \frac{1}{2} v_{XY} |F(X,Y)|^2 \right] dX$$

$$= \operatorname{Tr} \left[K_Y M_Y^{-1} \right] \int D_n(X)^2 |F(X,Y)|^2 dX. \tag{23}$$

The $n \times n$ matrices K_Y and M_Y are given by (20) and (22), with $\phi_{\alpha}(x)$ being the lowest n Dirichlet eigenfunctions of $-\Delta$, and with $h(x) = \prod_j f(x - y_j)$ and

$$|k(x)|^2 = |\nabla_x \prod_j f(x - y_j)|^2 + \frac{1}{2} \sum_j v(x - y_j) \prod_j f(x - y_j)^2,$$

respectively. Since K_Y is a positive definite matrix, we have the bound $\operatorname{Tr} K_Y M_Y^{-1} \leq \|M_Y^{-1}\| \operatorname{Tr} K_Y$, where $\|\cdot\|$ denotes the matrix norm (i.e., the largest eigenvalue for hermitian matrices). To calculate $\operatorname{Tr} K_Y$, and to bound $\|M_Y^{-1}\|$, we can assume that all the y_j 's are separated by at least a distance s, because the integrand of term II in (17) vanishes otherwise. Since $s \geq 2R$ by assumption, we have in this case

$$|k(x)|^2 = \left|\nabla_x \prod_j f(x - y_j)\right|^2 + \frac{1}{2} \sum_j v(x - y_j) \prod_j f(x - y_j)^2 = \sum_{j=1}^n \xi(x - y_j)$$
 (24)

with

$$\xi(x) = |\nabla f(x)|^2 + \frac{1}{2}v(x)f(x)^2. \tag{25}$$

Hence, if $\varrho_n^{\rm D}(x)$ denotes the one-particle density of $D_n(X)$, we have

$$\operatorname{Tr} K_Y = \sum_{j=1}^n \varrho_n^{\mathrm{D}} * \xi(y_j),$$
 (26)

where * denotes convolution.

To bound $||M_V^{-1}||$, we use the following:

Lemma 2. Assume that $|y_i - y_j| \ge s \ge 2R$ for all $i \ne j$. Then

$$||1 - M_Y|| \le \text{const.}\left(\frac{aR^2}{s^3} + n^{2/3}\frac{s^2}{\ell^2}\right).$$
 (27)

Proof. Let $q(x) = 1 - \prod_j f(x - y_j)^2 \ge 0$. Then, for any *n*-dimensional vector |b| with components b_{α} ,

$$(b|1 - M_Y|b) = \int q(x) \Big| \sum_{\alpha} b_{\alpha} \phi_{\alpha}(x) \Big|^2 d^3x.$$

Hence, the question about the largest eigenvalue of $1 - M_Y$ translates into the question of how large the average potential energy for the potential q(x) can be for functions such as $\sum_{\alpha} b_{\alpha} \phi_{\alpha}(x)$ whose kinetic energy is bounded above by (const.) $n^{2/3}\ell^{-2}$, i.e., the Fermi energy for n particles.

Let \mathcal{B}_j denote the ball of radius s/2 around y_j . Note that all these balls are non-overlapping by assumption. Also, since $s \geq 2R$, q(x) = 0 if x is outside all the balls. For a given function $\phi(x)$, let ϕ_j denote the average of $\phi(x)$ in the ball \mathcal{B}_j . Moreover, let $\eta(x) = \phi(x) - \bar{\phi}_j$. By the Cauchy-Schwarz inequality $(a + b)^2 \leq 2(a^2 + b^2)$, we get the bound

$$\int_{\mathcal{B}_i} q(x) |\phi(x)|^2 d^3x \le 2 \int_{\mathcal{B}_i} q(x) |\eta(x)|^2 d^3x + 2|\phi_j|^2 \int_{\mathcal{B}_i} q(x) d^3x. \tag{28}$$

Note that $|\phi_j|^2 \le 6/(\pi s^3) \int_{\mathcal{B}_i} |\phi(x)|^2 d^3x$, again by the Cauchy-Schwarz inequality. Moreover, since $s \ge R$,

$$\int_{\mathcal{B}_i} q(x) \, d^3x = \int_{\mathbb{R}^3} (1 - f(x)^2) \, d^3x \le (4\pi/3)aR^2.$$

To obtain the last inequality, we used the definition of f(x) as well as the fact that $\varphi(x) \ge \max\{1 - a/|x|, 0\}$, as explained in the beginning of this section.

Note that $\eta(x)$ is a function whose average over the ball \mathcal{B}_j is zero. In other words, it is orthogonal to the constant function in \mathcal{B}_j . Hence, using the fact that $q(x) \leq 1$ and Poincaré's inequality [15],

$$\int_{\mathcal{B}_j} q(x) |\eta(x)|^2 d^3x \le \int_{\mathcal{B}_j} |\eta(x)|^2 d^3x \le \text{const. } s^2 \int_{\mathcal{B}_j} |\nabla \eta(x)|^2 d^3x.$$

In this last expression we can replace $\eta(x)$ by $\phi(x)$, of course, since they only differ by a constant. Summing over all the balls \mathcal{B}_i (and using that q(x) = 0 outside the balls), we thus obtain that, for any function $\phi(x)$,

$$\int_{\mathbb{R}^3} q(x) |\phi(x)|^2 \, d^3\!x \leq \text{const.} \left[\frac{a R^2}{s^3} \int_{\mathbb{R}^3} |\phi(x)|^2 \, d^3\!x + s^2 \int_{\mathbb{R}^3} |\nabla \phi(x)|^2 \, d^3\!x \right].$$

In the case in question, the kinetic energy of $\phi(x)$ is bounded by const. $n^{2/3}\ell^{-2}$. This finishes the proof of the lemma.

Since $0 \le M_Y \le 1$ as a matrix, this lemma implies that

$$||M_Y^{-1}|| = \frac{1}{1 - ||1 - M_Y||} \le A_n \equiv \frac{1}{1 - \text{const.} \left[aR^2/s^3 + n^{2/3}(s/\ell)^2 \right]},\tag{29}$$

provided the denominator is positive. By inserting (26) and (29) into (23), we see that, for fixed Y with $|y_i - y_j| \ge s$ for all $i \ne j$,

$$\int G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X, Y)|^2 + \frac{1}{2} v_{XY} F(X, Y)^2 \right] dX$$

$$\leq A_n \sum_{j=1}^n \varrho_n^{D} * \xi(y_j) \int D_n(X)^2 F(X, Y)^2 dX. \tag{30}$$

To be able later to compare this expression (30) with $\langle \Psi | \Psi \rangle$, we want to put $G_n(X)^2$ back into the integrand. For this purpose we need the following lemma, which compares the integrals with and without the factor $G_n(X)^2$.

Lemma 3. For any fixed Y,

$$\int D_n(X)^2 F(X,Y)^2 G_n(X)^2 dX$$

$$\geq \int D_n(X)^2 F(X,Y)^2 dX \left(1 - \text{const.} n^{8/3} || M_Y^{-1} ||^2 (s/\ell)^5 \right). \tag{31}$$

Proof. Since g(x) = 1 for $|x| \ge 2s$, we have

$$G_n(X)^2 \ge 1 - \sum_{i \le j}^n \theta(2s - |x_i - x_j|).$$
 (32)

Here θ denotes the Heaviside step function, i.e., $\theta(t) = 1$ for $t \geq 0$ and $\theta(t) = 0$ for t < 0. To evaluate the integral of the second term in (32), we need the two-particle density of the state $D_n(X)F(X,Y)$ for each fixed Y. By Lemma 1 above, and the fact that $f(x) \leq 1$, this density, when appropriately normalized, is bounded from above by $||M_Y^{-1}||^2 \varrho_n^{D,(2)}(x,x')$, where $\varrho_n^{D,(2)}(x,x')$ denotes the two-particle density of the determinantal state $D_n(X)$. In particular, by explicit computation one finds that this latter density satisfies the bound

$$\varrho_n^{D,(2)}(x,x') \le \text{const.} |x-x'|^2 (n/\ell^3)^{8/3}$$
 (33)

for some constant independent of n and ℓ . Hence we arrive at (31).

We note that it is the n-dependence in inequality (31) that forces us to choose the particle number to be small and makes it necessary to localize the particles into small boxes. We also emphasize the importance of the exponent 5 in (31), which stems from the fact that the two-particle density vanishes as $|x - x'|^2$ for x close to x'. Had we not taken this into account, we would get an error term of the order $n^2(s/\ell)^3$ in (31). Note that necessarily s > a, and hence this error would be huge if $n \gg (a^3\varrho)^{-1}$, which is demanded by (19). This also explains why it is not possible to treat F(X,Y) on the same footing as $G_n(X)$ and $G_m(Y)$, since the two-particle density only vanishes as $|x - x'|^2$ for particles with equal spin, unlike the situation for particles of unequal spin.

Let

$$B_n = \left(1 - \text{const.} \, n^{8/3} A_n^2 (s/\ell)^5\right)^{-1},$$

assuming that the term in parenthesis is positive. Applying Lemma 3 to inequality (30), we arrive at

$$\int G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \frac{1}{2} v_{XY} F(X,Y)^2 \right] D_m(Y) G_m(Y) dX dY
\leq A_n B_n \sum_{j=1}^n \int \varrho_n^{D} * \xi(y_j) D_m(Y)^2 D_n(X)^2 F(X,Y)^2 G_m(Y)^2 G_n(X)^2 dX dY.$$
(34)

Now we cannot bound $\varrho_n^{\mathrm{D}} * \xi(y)$ independently of y by simply using the supremum of $\varrho_n^{\mathrm{D}}(x)$, since this number will be strictly bigger than n/ℓ^3 , even in the thermodynamic limit. Instead, we repeat the above argument for the Y integration. We use $|G_m(Y)| \leq 1$, the Y-analogues of Lemma 1 and then Lemma 3 to put $G_m(Y)^2$ back in. Here, it is important to note that now the x_i 's are separated by at least a distance $s \geq 2R$. In this way we obtain

$$\int G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \frac{1}{2} v_{XY} F(X,Y)^2 \right] D_m(Y) G_m(Y) dX dY$$

$$\leq A_n B_n B_m \int D_m(Y)^2 D_n(X)^2 F(X,Y)^2 G_m(Y)^2 G_n(X)^2 \operatorname{Tr} \widehat{K}_X M_X^{-1} dX dY. \tag{35}$$

The matrix M_X is the same as before, with Y replaced by X (and n replaced by m, of course), and \widehat{K}_X is the $m \times m$ matrix

$$(\widehat{K}_X)_{\alpha\beta} = \int \phi_{\alpha}(y)^* \phi_{\beta}(y) \prod_i f(y - x_i)^2 \varrho_n^{\mathcal{D}} * \xi(y) d^3y.$$

Using $|f(x)| \le 1$ and $||M_X^{-1}|| \le A_m$, which follows from Lemma 2 and the fact that the x_i 's are separated at least by a distance s, we get the bound

$$\operatorname{Tr} \widehat{K}_X M_X^{-1} \le A_m \operatorname{Tr} \widehat{K}_X \le A_m \int \varrho_n^{\mathcal{D}}(x) \varrho_m^{\mathcal{D}}(y) \xi(x-y) \, d^3x \, d^3y. \tag{36}$$

We recall the definition of f(x) and the properties of $\varphi(x)$ stated in the beginning of this section to calculate the integral $\int \xi(y) d^3y = 4\pi a(1 - a/R)^{-1}$. We then use this information to bound the last integral in (36), by using Young's inequality [15]. Thus

$$\operatorname{Tr} \widehat{K}_X M_X^{-1} \le A_m \left(\int \varrho_n^{\mathcal{D}}(x)^2 \, d^3x \right)^{1/2} \left(\int \varrho_m^{\mathcal{D}}(y)^2 \, d^3y \right)^{1/2} 4\pi a (1 - a/R)^{-1}. \tag{37}$$

For the square of $\varrho_n^{\rm D}(x)$ we find

$$\int \varrho_n^{\rm D}(x)^2 d^3x = \frac{1}{\ell^3} \sum_{p,q} \prod_{a=1}^3 \left(1 + \frac{1}{2} \delta_{p_a,q_a} \right), \tag{38}$$

where p_a denotes the components of the wave vector p, and the sums are over the n lowest eigenstates of the Dirichlet Laplacian, $(2/\ell)^{3/2} \prod_{a=1}^{3} \sin(p_a x_a)$. From this explicit expression it is easy to see that

$$\int \varrho_n^{\rm D}(x)^2 \, d^3x \le \frac{n^2}{\ell^3} \left(1 + \text{const.} \, n^{-1/3} \right). \tag{39}$$

The same holds with n replaced by m. Eq. (35) thus implies the upper bound

$$\int G_n(X)^2 D_n(X)^2 \left[|\nabla_X F(X,Y)|^2 + \frac{1}{2} v_{XY} F(X,Y)^2 \right] D_m(Y) G_m(Y) dX dY
\leq \langle \Psi | \Psi \rangle \frac{4\pi a n m}{\ell^3} A_n A_m B_n B_m (1 - a/R)^{-1} \left(1 + \text{const.} \, n^{-1/3} + \text{const.} \, m^{-1/3} \right).$$
(40)

The same bound holds, of course, with X and Y interchanged. We therefore have the upper bound

$$II \le \langle \Psi | \Psi \rangle \frac{8\pi a n m}{\ell^3} A_n A_m B_n B_m (1 - a/R)^{-1} \left(1 + \text{const. } n^{-1/3} + \text{const. } m^{-1/3} \right). \tag{41}$$

It remains to bound the term III. Using $|g(x)| \leq 1$ we have that

$$|\nabla_X G_n(X)|^2 \le \sum_{i=1}^n \sum_{j, j \neq i} |\nabla g(x_i - x_j)|^2 + \sum_{i=1}^n \sum_{j, j \neq i} \sum_{k, k \neq i, j} |\nabla g(x_i - x_j)| |\nabla g(x_i - x_k)|.$$
(42)

Now, by Lemma 1, the appropriately normalized k-particle densities of $D_n(X)F(X,Y)$ are bounded above by $\|M_Y^{-1}\|^k \varrho_n^{\mathrm{D},(k)}$, where $\varrho_n^{\mathrm{D},(k)}$ denotes the k-particle density of $D_n(X)$. In particular, $\varrho_n^{\mathrm{D},(2)}$ is satisfies the bound (33), and $\varrho_n^{\mathrm{D},(3)}$ satisfies

$$\varrho_n^{D,(3)}(x, x', x'') \le \text{const.} (n/\ell^3)^3$$

for some constant independent of n and ℓ . Using the fact that $\nabla g(x)$ is supported on the set $|x| \leq 2s$, together with $|\nabla g(x)| \leq \text{const. } s^{-1}$, we obtain from (42), for any fixed Y,

$$\int D_n(X)^2 F(X,Y)^2 |\nabla_X G_n(X)|^2 dX$$

$$\leq \text{const. } \frac{n^2}{\ell^3} s \left(\|M_Y^{-1}\|^2 n^{2/3} (s/\ell)^2 + \|M_Y^{-1}\|^3 n (s/\ell)^3 \right) \int D_n(X)^2 F(X,Y)^2 dX. \tag{43}$$

Finally, to get a bound on III, we proceed as above, using (29) (and the fact that the y_j 's are separated by a distance s) and Lemma 3 to put $G_n(X)^2$ back into the integral. Note, however, that it is enough to bound A_n and B_n by constants in this term. Assuming that $n(s/\ell)^3$ is small, the second term in the parenthesis in (43) is negligible compared to the first term. The same bound applies to the case where X and Y are interchanged, and hence we obtain

$$III \le \langle \Psi | \Psi \rangle \operatorname{const.} \left(n^{8/3} + m^{8/3} \right) \frac{s^3}{\ell^5}. \tag{44}$$

Collecting all the error terms obtained in Eqs. (19), (41) and (44) and inserting them into (14) and (15), we obtain

$$E_{0}(n,m,\ell) \leq \frac{3}{5} (6\pi^{2})^{2/3} \frac{n^{5/3} + m^{5/3}}{\ell^{2}} \left(1 + Cn^{-1/3} + Cm^{-1/3} \right)$$

$$+8\pi a \frac{nm}{\ell^{3}} \left(1 + \varepsilon + C \left[\frac{aR^{2}}{s^{3}} + (n+m)^{2/3} (s/\ell)^{2} + \frac{a}{R} + \frac{1}{n^{1/3}} + \frac{1}{m^{1/3}} + (n+m)^{8/3} (s/\ell)^{5} \right] \right)$$

$$+ \frac{Cs}{\varepsilon} \frac{(n+m)^{2}}{\ell^{3}} \left[(n+m)^{2/3} (s/\ell)^{2} \right]$$

$$(45)$$

for some constant C > 0. In Ineq. (45) we have assumed smallness of all the error terms, i.e., that the terms in square brackets are small. This condition will be fulfilled, at low density, with our choice of R, s, n, m and ℓ below.

The optimal choice of ε in (45) is given by $\varepsilon^2 = \text{const.} (n+m)^{8/3} s^3/(\ell^2 anm)$. Inserting this value for ε we infer from (45)

$$E_{0}(n,m,\ell) \leq \frac{3}{5}(6\pi^{2})^{2/3}\frac{n^{5/3}+m^{5/3}}{\ell^{2}}\left(1+Cn^{-1/3}+Cm^{-1/3}\right) +8\pi a\frac{nm}{\ell^{3}}\left(1+C\left[\frac{aR^{2}}{s^{3}}+(n+m)^{2/3}(s/\ell)^{2}+\frac{a}{R}+\frac{1}{n^{1/3}}+\frac{1}{m^{1/3}}+(n+m)^{8/3}(s/\ell)^{5}\right]\right) +C(n+m)^{7/3}\frac{s^{3/2}a^{1/2}}{\ell^{4}}.$$

$$(46)$$

Eq. (46) is our final bound on the energy $E_0(n, m, \ell)$. To apply this result in (10) we have to insert the values (9) for n and m. Recall that $|n - \varrho_1(\ell + R_0)^3| \le 1$ and $|m - \varrho_2(\ell + R_0)^3| \le 1$. We are then still free to choose R, s and ℓ . We choose

$$R = a(a\varrho^{1/3})^{-2/9}$$
, $s = 2R$, $\ell = \varrho^{-1/3}(a\varrho^{1/3})^{-11/9}$.

Inserting these values into (46) we thus obtain, for small ϱ ,

$$\frac{1}{\ell^3} E_0(n, m, \ell) \le \frac{3}{5} (6\pi^2)^{2/3} \left[\varrho_1^{5/3} + \varrho_2^{5/3} \right] + 8\pi a \varrho_1 \varrho_2 + \text{const. } a \varrho^2 \left(a \varrho^{1/3} \right)^{2/9}.$$

In combination with Eq. (10), this finishes the proof of the upper bound. Note that the contribution to the error term that arises from the fact that $E_0(n, m, \ell)$ has to be divided by $(\ell + 2R_0)^3$ and not ℓ^3 in (10), is of the order $\varrho^{5/3}R_0/\ell$ and, for this choice of ℓ , is much smaller than $a\varrho^2(a\varrho^{1/3})^{2/9}$ when ϱ is small.

V. LOWER BOUND TO THE GROUND STATE ENERGY

A. The Dyson Lemma

We start with a generalization of a lemma of Dyson [6], which bounds the hard potential v(x) (which may or may not contain a hard core) from below by a soft potential U(x), at the expense of using up some positive kinetic energy. In the following, $\hat{f}(k)$ denotes the Fourier transform of a function f(x), i.e., $\hat{f}(k) = (2\pi)^{-3/2} \int f(x) \exp(ik \cdot x) d^3x$. Dyson's result was generalized in [5] and it is further generalized here by separating low from high momentum. In our application "low" will mean $\varrho^{1/3}$ and "high" will mean 1/a. The analogous inequality for 2D is stated as Lemma 7 below. The proof of both lemmas is given in the appendix.

Lemma 4. For $R > R_0$, let $\theta_R(x)$ denote the characteristic function of a ball of radius R centered at the origin, i.e., $\theta_R(x) = 1$ if |x| < R and = 0 otherwise. Let $\chi(p)$ be a radial function, $0 \le \chi(p) \le 1$, such that $h(x) \equiv \widehat{(1-\chi)}(x)$ is bounded and integrable. Let

$$f_R(x) = \sup_{|y| \le R} |h(x - y) - h(x)|,\tag{47}$$

and

$$w_R(x) = \frac{2}{\pi^2} f_R(x) \int_{\mathbb{R}^3} f_R(y) \, d^3y.$$
 (48)

Then, for any positive, radial function U(x), supported in the annulus $R_0 \le |x| \le R$, with $\int_{\mathbb{R}^3} U(x) d^3x = 4\pi$, and for any $\varepsilon > 0$,

$$-\nabla \chi(p)\theta_R(x)\chi(p)\nabla + \frac{1}{2}v(x) \ge (1-\varepsilon)aU(x) - \frac{a}{\varepsilon}w_R(x). \tag{49}$$

Here, $\theta_R(x)$ is multiplication operator in x-space, whereas $\chi(p)$ is a multiplication operator in momentum space. Thus, $\nabla \chi(p)\theta_R(x)\chi(p)\nabla$ is an operator version of ∇^2 , which is cut off in both configuration and in momentum spaces.

The original Dyson lemma (as modified in [5]) has $\chi(p) \equiv 1$ and $w_R(x) \equiv 0$, i.e., there is no cutoff. The cutoff $\chi(p)$ in (49) essentially says that only the high momentum part of ∇ is needed to give a good account of the scattering of two particles. The (relatively) low momentum part of ∇ is not used in (49) and is thereby saved for later use to give a good estimate of the part of the fermion kinetic energy needed to fill the Fermi sea. The price we pay for this luxury is the error term $aw_R(x)/\varepsilon$, which does not appear in Dyson's lemma.

Note that, by construction, either $w_R(x)$ is bounded and integrable or else $w_R(x) = \infty$ for all x. If $\chi(p) \equiv 1$, then $w_R(x) \equiv 0$, and hence we can set $\varepsilon = 0$ to recover the Dyson Lemma in [5], which says that for any $\phi(x)$, $\int_{|x| < R} (|\nabla \phi(x)|^2 + [\frac{1}{2}v(x) - aU(x)]|\phi(x)|^2) d^3x \ge 0.$

Corollary 1. If $y_1, ..., y_N$ denote N points in \mathbb{R}^3 , with $|y_i - y_j| \ge 2R$ for all $i \ne j$, then, as an operator on functions of x,

$$-\nabla \chi(p)^2 \nabla + \frac{1}{2} \sum_{i=1}^N v(x - y_i) \ge \sum_{i=1}^N \left((1 - \varepsilon) a U(x - y_i) - \frac{a}{\varepsilon} w_R(x - y_i) \right). \tag{50}$$

Proof. This follows immediately from the previous lemma, using translation invariance and the fact that $\sum_i \theta_R(x - y_i) \le 1$ since all the balls are non-overlapping, by assumption.

To apply this corollary, let l(p) be a smooth, radial, positive function with l(p) = 0 for $|p| \le 1$, l(p) = 1 for $|p| \ge 2$, and $0 \le l(p) \le 1$ in-between. For some s > 0 let

$$\chi_s(p) = l(sp). \tag{51}$$

Note that with this choice of $\chi_s(p)$ the corresponding $h(x) = \widehat{1-\chi_s}(x)$ is a smooth function of rapid decay and hence, by simple scaling, the corresponding potential $w_R(x)$ satisfies (for $R \leq \text{const. } s$)

$$|w_R(x)| \le \text{const.} \frac{R^2}{s^5}$$
 and $\int |w_R(x)| d^3x \le \text{const.} \frac{R^2}{s^2}$ (52)

for some constants depending only on l. Moreover, if $|y_i - y_j| \ge 2R$ for all $i \ne j$, then

$$\sum_{i=1}^{N} w_R(x - y_i) \le \text{const.} \frac{1}{Rs^2}$$

$$(53)$$

independent of x and N. Later we are going to choose $R \ll s \ll \varrho^{-1/3}$ (cf. Eq. (72)).

B. A priori bounds

For $N_1 + N_2 = N$, let $\Psi_N(X, Y)$ be a sequence of normalized wave functions, antisymmetric both in the X and in the Y variables. We assume that $N_1/L^3 \to \varrho_1$ and $N_2/L^3 \to \varrho_2$ as $N \to \infty$, with $\varrho = \varrho_1 + \varrho_2$. Let γ_1 and γ_2 denote

the reduced one-particle density matrices of $\Psi_N(X,Y)$ for the X- and Y-particles, respectively, with $\operatorname{Tr} \gamma_1 = N_1$ and $\operatorname{Tr} \gamma_2 = N_2$. Moreover, let P_M denote the following spectral projection of the Laplacian with *periodic* boundary conditions on Λ , given by the integral kernel

$$P_M(x, x') = \frac{1}{L^3} \sum_{\substack{p \in (2\pi/L)\mathbb{Z}^3 \\ |p| \le (6\pi^2 M/L^3)^{1/3}}} e^{ip \cdot (x - x')}$$
(54)

for $x, x' \in \Lambda$. Note that, by scaling, $\text{Tr}[P_M]$ does not depend on L, and

$$\lim_{m \to \infty} \frac{1}{M} \operatorname{Tr} \left[P_M \right] = 1. \tag{55}$$

In Lemmas 5 and 6 we derive some bounds for sequences of wave functions satisfying certain energy bounds. These lemmas apply, in particular, to the true ground state – as shown in the previous section. We call these bounds a priori bounds.

Lemma 5. Assume that, in the thermodynamic limit $(N \to \infty, L \to \infty \text{ with } \varrho_i = N_i/L^3 \text{ fixed})$, there is a sequence of states $\Psi_N(X,Y)$ such that

$$\limsup_{L \to \infty} \frac{1}{L^3} \langle \Psi_N | H | \Psi_N \rangle \le \frac{3}{5} \left(6\pi^2 \right)^{2/3} \left[\varrho_1^{5/3} + \varrho_2^{5/3} \right] + Ca\varrho^2 \tag{56}$$

for some C > 0 independent of ϱ . Then, for i = 1, 2 (and with γ_1, γ_2 being the one-body density matrices),

$$\limsup_{L \to \infty} \frac{1}{L^3} \operatorname{Tr} \left[\gamma_i (1 - P_{N_i}) \right] \le \operatorname{const.} \varrho \sqrt{a \varrho^{1/3}}. \tag{57}$$

Proof. We immediately have the trivial lower bound for non-interacting fermions

$$\liminf_{L \to \infty} \frac{1}{L^3} \langle \Psi_N | -\Delta_X - \Delta_Y | \Psi_N \rangle \ge \frac{3}{5} \left(6\pi^2 \right)^{2/3} \left[\varrho_1^{5/3} + \varrho_2^{5/3} \right]. \tag{58}$$

To prove Ineq. (57), however, we need the following refinement of (58), which is proved in [16, Eq. (4.13)]:

$$\liminf_{L \to \infty} \frac{1}{L^3} \langle \Psi_N | -\Delta_X - \Delta_Y | \Psi_N \rangle \ge \frac{3}{5} \left(6\pi^2 \right)^{2/3} \limsup_{N \to \infty} \left[\varrho_1^{5/3} (1 + \text{const. } \zeta_1^2) + \varrho_2^{5/3} (1 + \text{const. } \zeta_2^2) \right], \tag{59}$$

where $\zeta_i = N_i^{-1} \text{Tr} \left[\gamma_i (1 - P_{N_i}) \right]$ for i = 1, 2. Using (56) as well as the fact that the interaction potential is assumed to be positive, we immediately obtain (57).

Our second a priori bound concerns the nearest neighbor distance among particles. For given points y_1, \ldots, y_{N_2} in \mathbb{R}^3 , let $I_R(y_1, \ldots, y_{N_2})$ be the number of y_i 's with the property that the distance to the nearest neighbor among the other y_i 's is less than 2R.

Lemma 6. Assume that there exists a C > 0, independent of $\varrho = N/L^3$, such that

$$\frac{1}{N} \langle \Psi_N | H | \Psi_N \rangle \le C \varrho^{2/3}. \tag{60}$$

Then

$$\langle \Psi_N | I_R(y_1, \dots, y_{N_2}) | \Psi_N \rangle \le \text{const. } N(R^3 \varrho)^{2/3}.$$
 (61)

Proof. With δ_i denoting the distance to the nearest neighbor, we have

$$I_R(y_1, \dots, y_{N_2}) \le (2R)^2 \sum_{i=1}^{N_2} \frac{1}{\delta_i^2}.$$

The result now follows from the operator inequality

$$\sum_{i=1}^{N_2} \frac{1}{\delta_i^2} \le \text{const.} \sum_{i=1}^{N_2} -\Delta_i \tag{62}$$

which holds on anti-symmetric wave functions of N_2 variables, and is proved in [17, Thm. 5]. Note that we again used the fact that the interaction potential is positive, and hence the kinetic energy is bounded above by the total energy.

C. Putting it together

For a lower bound, we can neglect the interaction among particles of the same kind. That is, we use

$$H \ge \left(-\Delta_X + \frac{1}{2}v_{XY}\right) + \left(-\Delta_Y + \frac{1}{2}v_{XY}\right). \tag{63}$$

We are going to bound both terms separately using the *a priori* bounds of the previous section. In the following, we are going to treat only the first term, the lower bound on the second term can be obtained in the same way by exchanging X and Y.

First, we decompose the Laplacian into a high and a low momentum part, as follows:

$$\Delta = \nabla \Gamma(p) \nabla + \nabla (1 - \Gamma(p)) \nabla.$$

For $\varrho = N/L^3$, let $k_{\rm F} = (6\pi^2\varrho)^{1/3}$ be the Fermi momentum (for spinless fermions), and let

$$\Gamma(p) = \max \left\{ 1 - \frac{k_{\rm F}^2}{|p|^2}, 0 \right\}.$$

We claim that

$$\sum_{i=1}^{N_1} -\nabla_i \left(1 - \Gamma(p_i)\right) \nabla_i \ge \frac{3}{5} \left(6\pi^2\right)^{2/3} \frac{N_1^{5/3}}{L^2}.$$
 (64)

To show this, we use the argument in [18]. Let $\phi_i(x)$, $i = 1, ..., N_1$, be any set of orthonormal functions with support in the cube Λ of side length L. We want a lower bound to the expression

$$\sum_{i=1}^{N_1} \int_{\mathbb{R}^3} |p|^2 \left(1 - \Gamma(p)\right) |\widehat{\phi}_i(p)|^2 d^3 p.$$
 (65)

Note that $\widehat{\phi}_i(p) = (2\pi)^{-3/2} \langle e^{ip\cdot x} | \phi_i \rangle$, with $\langle \cdot | \cdot \rangle$ denoting the inner product for functions on the cube Λ . Since the $\phi_i(x)$ are orthonormal, we have that

$$\sum_{i=1}^{N_1} |\widehat{\phi}_i(p)|^2 \le (2\pi)^{-3} \langle e^{ip \cdot x} | e^{ip \cdot x} \rangle = (2\pi)^{-3} L^3.$$

Hence (65) is bounded below by the infimum of $\int p^2 (1 - \Gamma(p)) \, \xi(p) \, d^3p$ over all $0 \le \xi(p) \le (2\pi)^{-3} L^3$ with $\int \xi(p) \, d^3p = N_1$. Since $|p|^2 (1 - \Gamma(p))$ is a monotone increasing function of |p|, the infimum is attained by $\xi(p) = \theta((6\pi^2 N_1/L^3)^{1/3} - (6\pi^2 N_1/L^3)^{1/3})$

|p|), with θ denoting the Heaviside step function. Now $\Gamma(p)=0$ for $|p|\leq (6\pi^2N_1/L^3)^{1/3}\leq (6\pi^2\varrho)^{1/3}$, and thus we arrive at (64).

For the high-momentum part, we use that

$$\Gamma(p) \ge \left(1 - s^2 k_{\rm F}^2\right) \chi_s(p)^2$$

for any $s \leq 1/k_{\rm F}$, with $\chi_s(p)$ defined in (51). Hence, we can use Corollary 1 to get a lower bound on this term. In order to be able to apply this corollary, however, we have to make sure that the y_j 's are separated at least a distance 2R. Let $\widetilde{Y} \subset Y$ be the set of y_j 's whose distance to the nearest neighbor is at least 2R. Note that, by definition, $|\widetilde{Y}| = N_2 - I_R(Y)$. We are going to neglect the interaction with y_j 's that are not in the set \widetilde{Y} , which can only lower the energy. Hence we obtain, for a given configuration of Y,

$$\sum_{i=1}^{N_1} -\nabla_i \Gamma(p_i) \nabla_i + \frac{1}{2} \sum_{i,j} v(x_i - y_j) \ge (1 - s^2 k_F^2) \sum_{i=1}^{N_1} W_Y(x_i),$$

with

$$W_Y(x) = \sum_{\{j: y_j \in \widetilde{Y}\}} \left((1 - \varepsilon) a U(x - y_j) - \frac{a}{\varepsilon} w_R(x - y_j) \right), \tag{66}$$

depending on ε , a, R and s.

We are still free to choose U(x). A convenient choice is

$$U(x) = \begin{cases} 3\left(R^3 - R_0^3\right)^{-1} & \text{for } R_0 \le |x| \le R\\ 0 & \text{otherwise,} \end{cases}$$

but any other choice such that $|U(x)| \leq \text{const.} R^{-3}$ for $R \gg R_0$ will do for our purpose.

Now let $\Psi_N(X,Y)$ be a normalized fermionic wave function. We can express the expectation value of $\sum_i W_Y(x_i)$ as

$$\left\langle \Psi_N \left| \sum_{i=1}^{N_1} W_Y(x_i) \right| \Psi_N \right\rangle = \int n_Y \text{Tr} \left[\gamma_Y W_Y \right] dY, \tag{67}$$

where

$$n_Y = \int |\Psi_N(X, Y)|^2 dX \tag{68}$$

and γ_Y denotes the one-particle density matrix of $\Psi_N(X,Y)$ for fixed Y, i.e.,

$$\gamma_Y(x, x') = \frac{N_1}{n_Y} \int \Psi_N(x, x_2, \dots, x_{N_1}, Y) \Psi_N(x', x_2, \dots, x_{N_1}, Y)^* d^3x_2 \cdots d^3x_{N_1}.$$
 (69)

Note that $0 \le \gamma_Y \le 1$ and $\operatorname{Tr} \gamma_Y = N_1$. Moreover, $\int n_Y dY = 1$ and $\int n_Y \gamma_Y dY = \gamma_1$, the one-particle reduced density matrix for the X-particles.

Let P be a projection operator, and let γ denote any fermionic density matrix, which is an operator that satisfies $0 \le \gamma \le 1$ and $\operatorname{Tr} \gamma = N_1$. Let W_{\pm} be two bounded positive semi-definite operators, and let $W = W_+ - W_-$. For any $\delta > 0$, we have

$$\operatorname{Tr} [\gamma W] = \operatorname{Tr} [PW] + \operatorname{Tr} [(\gamma - 1)PWP]$$

$$+ \operatorname{Tr} [\gamma ((1 - P)WP + PW(1 - P) + (1 - P)W(1 - P))]$$

$$\geq \operatorname{Tr} [PW_{+}](1 - \delta) - \operatorname{Tr} [PW_{-}](1 + \delta)$$

$$- (1 + \delta^{-1}) (\|W_{+}\| + \|W_{-}\|) \operatorname{Tr} [\gamma (1 - P)] - \|W\| \operatorname{Tr} [P(1 - \gamma)],$$

with $\|\cdot\|$ denoting operator norm. Now let $P \equiv P_{N_1}$ be the operator defined in (54), and $W = W_Y$. We choose W_+ to be the terms in (66) containing U(x), and W_- the ones containing $w_R(x)$. We then have, using $\int U(x) d^3x = 4\pi$,

$$\operatorname{Tr}[PW_{+}] = \frac{\operatorname{Tr}[P_{N_{1}}]}{L^{3}} \sum_{\{j: y_{j} \in \widetilde{Y}\}} (1 - \varepsilon) a \int_{[0,L]^{3}} U(x - y_{j}) d^{3}x$$

$$\geq \frac{\operatorname{Tr}[P_{N_{1}}]}{L^{3}} (1 - \varepsilon) 4\pi a \left[N_{2} - I_{R}(Y) - \operatorname{const.} \frac{L^{2}}{R^{2}} \right].$$

The last term in square brackets bounds the number of y_j 's in \widetilde{Y} that are at least a distance R away from the boundary of the box. Since the distance between the y_j 's is bigger than 2R by assumption, the number of such y_j 's close to the boundary is bounded by const. L^2/R^2 . By Lemma 6,

$$\int n_Y I_R(Y) dY = \langle \Psi_N | I_R(Y) | \Psi_N \rangle \le \text{const. } N(R^3 \varrho)^{2/3}$$
(70)

if $\Psi_N(X,Y)$ is an approximate ground state. As already noted in Eq. (55), $\text{Tr}[P_{N_1}]$ can be replaced by N_1 in the thermodynamic limit.

Analogously, using (52), we get an upper bound

$$\operatorname{Tr}\left[PW_{-}\right] \leq \operatorname{const.} \frac{aR^{2}}{\varepsilon s^{2}} \frac{N_{2}\operatorname{Tr}\left[P_{N_{1}}\right]}{L^{3}}.$$

Moreover, using (53) and the fact that the distance between y_i 's contributing to W_Y is at least 2R, we find that

$$||W_Y||_{\infty} \le ||W_+|| + ||W_-|| \le \left(\frac{3a}{R^3 - R_0^3} + \text{const.} \frac{a}{\varepsilon s^2 R}\right).$$

The a priori bound in Lemma 5 implies that, for large enough N,

$$\int n_Y \text{Tr} \left[\gamma_Y (1 - P) \right] dY = \text{Tr} \left[\gamma_1 (1 - P) \right] \le C N (a^3 \varrho)^{1/6}, \tag{71}$$

where γ_1 is the one-particle density matrix (for the X-particles) of any approximate ground state. The same bound is true for $\text{Tr}\left[P(1-\gamma_1)\right] = \text{Tr}\left[\gamma_1(1-P)\right] + \text{Tr}\left[P-\gamma_1\right]$, since $N_1^{-1}\text{Tr}\left[P-\gamma_1\right] \to 0$ as $N_1 \to \infty$ (see (55)). Hence, collecting all the bounds, and applying the same arguments also to the second term in (63), we arrive at the lower bound

$$\lim_{L \to \infty} \frac{1}{L^3} E_0(N_1, N_2, L) \ge \frac{3}{5} \left(6\pi^2\right)^{2/3} \left[\varrho_1^{5/3} + \varrho_2^{5/3}\right] \\
+8\pi a \varrho_1 \varrho_2 \left(1 - \varepsilon - \delta - s^2 (6\pi^2 \varrho)^{2/3} - C \frac{R^2}{\varepsilon s^2}\right) - C a \varrho^2 (R^3 \varrho)^{2/3} \\
-C \varrho (a^3 \varrho)^{1/6} \left(1 + \frac{1}{\delta}\right) \left(\frac{a}{R^3 - R_0^3} + \frac{a}{\varepsilon s^2 R}\right)$$

for some C > 0.

We choose

$$R = \varrho^{-1/3} (a\varrho^{1/3})^{3/26} , \ s = \varrho^{-1/3} (a\varrho^{1/3})^{1/26} , \ \varepsilon = \delta = (a\varrho^{1/3})^{1/13}$$
 (72)

and obtain, for small ϱ ,

$$\lim_{L \to \infty} \frac{1}{L^3} E_0(N_1, N_2, L) \ge \frac{3}{5} \left(6\pi^2\right)^{2/3} \left[\varrho_1^{5/3} + \varrho_2^{5/3}\right] + 8\pi a \varrho_1 \varrho_2 - \text{const. } a\varrho^2 \left(a\varrho^{1/3}\right)^{1/13}.$$

This finishes the proof of the lower bound.

VI. THE TWO-DIMENSIONAL GAS

We now comment on the necessary changes in considering the 2D gas instead of the 3D gas. We start with the lower bound to the ground state energy. The analogue of Lemma 4 in 2D is the following lemma, which generalizes the corresponding result used for bosons in 2D in [9]. Its proof can again be found in the appendix.

Lemma 7. For $R > R_0$, let $\theta_R(x)$ denote the characteristic function of a disc of radius R centered at the origin, i.e., $\theta_R(x) = 1$ if |x| < R and = 0 otherwise. Let $\chi(p)$ be a radial function, $0 \le \chi(p) \le 1$, such that $h(x) \equiv \widehat{(1-\chi)}(x)$ is bounded and integrable. Let

$$f_R(x) = \sup_{|y| \le R} |h(x - y) - h(x)|,\tag{73}$$

and

$$w_R(x) = \frac{2}{\pi} f_R(x) \int_{\mathbb{R}^2} f_R(y) \, d^2 y. \tag{74}$$

Let U(x) be any positive, radial function, supported in the annulus $R_0 \leq |x| \leq R$, with

$$\int_{\mathbb{R}^2} U(x) \ln(|x|/a) \, d^2x = 2\pi. \tag{75}$$

Then, for any $\varepsilon > 0$,

$$-\nabla \chi(p)\theta_R(x)\chi(p)\nabla + \frac{1}{2}v(x) \ge (1-\varepsilon)U(x) - \frac{1}{\varepsilon} \left[(2\pi)^{-1} \int U(y) \, d^2y \right] w_R(x). \tag{76}$$

In the application, we choose, as in [9],

$$U(x) = \begin{cases} \nu(R)^{-1} & \text{for } R_0 \le |x| \le R\\ 0 & \text{otherwise,} \end{cases}$$
 (77)

with $\nu(R)$ determined by condition (75), i.e.,

$$\nu(R) = \int_{R_0}^R \ln(r/a)r \, dr = \frac{1}{4} \left[R^2 \ln \frac{R^2}{a^2 e} - R_0^2 \ln \frac{R_0^2}{a^2 e} \right]. \tag{78}$$

Using that $a \leq R_0 \leq R$ we get the bounds

$$\frac{1}{2}(R^2 - R_0)^2 \left(\ln R/a - \frac{1}{2}\right) \le \nu(R) \le \frac{1}{2}R^2 \ln R/a,\tag{79}$$

from which, in turn, we get upper and lower bounds on $\int U(x) d^2x = \nu(R)^{-1} \pi (R^2 - R_0^2)$.

Moreover, we again choose $\chi(p)$ as in (51), with $R \leq \text{const.} s$. Inequalities (52)–(53) then have to be replaced in the 2D case by

$$|w_R(x)| \le \text{const.} \frac{R^2}{s^4}$$
 and $\int |w_R(x)| d^2x \le \text{const.} \frac{R^2}{s^2}$ (80)

and

$$\sum_{i=1}^{N} w_R(x - y_i) \le \text{const.} \frac{1}{s^2}$$
(81)

in case that $|y_i - y_j| \ge 2R$ for all $i \ne j$.

The *a priori* bounds of Subsect. VB can be obtained also in the 2D case. The proof of Lemma 5 works in the same way, with the appropriate changes in the expression of the kinetic and interaction energy, of course. For the proof of Lemma 6, we note that the analogue of the inequality (62) does *not* hold in 2 dimensions. However, a 'relativistic' version of it is true, namely that

$$\sum_{i=1}^{N_2} \frac{1}{\delta_i} \le \text{const.} \sum_{i=1}^{N_2} \sqrt{-\Delta_i}$$
(82)

on antisymmetric functions of N_2 variables $y_i \in \mathbb{R}^2$. Ineq. (82) can be proved in a similar way as the proof of (62) in [17]. It implies that

$$\langle \Psi_N | I_R(y_1, \dots, y_{N_2}) | \Psi_N \rangle \le 2R \operatorname{Tr} \left[\sqrt{-\Delta} \gamma \right] \le 2R \left(\operatorname{Tr} \left[-\Delta \gamma \right] \right)^{1/2} \left(\operatorname{Tr} \gamma \right)^{1/2} \le \operatorname{const.} N(R^2 \varrho)^{1/2}$$
(83)

in 2D, replacing (61). Here γ denotes the one-particle density matrix (for the Y particles) of $\Psi_N(X, Y)$, and we have used Schwarz's inequality as well as the assumption $\text{Tr}\left[-\Delta\gamma\right] \leq \text{const. } N\varrho$ for an approximate ground state.

With the *a priori* bounds in hand, we can proceed along the same lines as in Subsect. V C to obtain a lower bound to the ground state energy. The optimal choice of the free parameters ε , δ , R and s in 2D turns out to be

$$R = \varrho^{-1/2} \frac{1}{|\ln(a^2 \varrho)|^{3/20}} , \ s = \varrho^{-1/2} \frac{1}{|\ln(a^2 \varrho)|^{1/20}} , \ \varepsilon = \delta = \frac{1}{|\ln(a^2 \varrho)|^{1/10}}.$$

This yields the lower bound in Theorem 2.

Our last task is to derive the upper bound in Theorem 2. It turns out that obtaining this bound is actually much easier than in the 3D case. The reason for the rather complicated construction in 3D was the very small interaction energy $\sim a\varrho$ per particle, which forced us to choose the particle number in a box to be quite large, namely $n \gg 1/(a^3\varrho)$, in order to have negligible finite size effects. This resulted in a trial wave function with very small norm. In 2D, however, it is possible to choose the particle number in each box much smaller, such that the norm of the trial wave function is close to one. If we take the analogous function as in (11)–(12), with s=2R and with $\varphi(x)$ now being the solution to the zero-energy scattering equation in 2D, cut off at an appropriate radius R, then a simple bound as in the proof of Lemma 3 shows that

$$\langle \psi | \psi \rangle \ge 1 - \text{const.} \, n(R^2 \rho).$$
 (84)

Hence we have to choose the box size ℓ and R such that $nR^2\varrho^2\ll 1$, with $n\sim \varrho\ell^2$. Moreover, the restriction on having a negligible finite size effect is $n^{1/2}\gg |\ln(a^2\varrho)|$ (compare with (19)). If we choose $R=\varrho^{-1/2}|\ln(a^2\varrho)|^{-\alpha}$ for large enough α , then all these conditions are easily fulfilled. In calculating the kinetic energy in (17) and (18), we can then just use the simple bounds $g(x)\leq 1$ and $f(x)\leq 1$. We demonstrate this on the analogue of the term II in (17) in 2D. Namely, with $\xi(x)$ given as in (25),

$$\int \left[|\nabla_X F(X,Y)|^2 + \frac{1}{2} v_{XY} F(X,Y)^2 \right] D_n(X)^2 D_m(Y)^2 G_n(X)^2 G_m(Y)^2 dX dY
\leq \sum_{i=1}^n \sum_{j=1}^m \int \xi(x_i - y_j) D_n(X) D_m(Y) dX dY = \int \varrho_n^{\mathrm{D}}(x) \varrho_m^{\mathrm{D}}(y) \xi(x - y) d^3x d^3y.$$
(85)

Here we have also used the fact that the integrand vanishes whenever two particles of the same kind are closer together then a distance $s \ge 2R$, in order for (24) to hold. We can then proceed using Young's inequality on the last term, as

in (37)–(39). The leading term from the interaction energy then comes from

$$\int_{|x| \le R} (|\nabla \varphi(x)|^2 + \frac{1}{2}v(x)|\varphi(x)|^2) \, d^2x = \frac{2\pi}{\ln(R/a)} \le \frac{4\pi}{|\ln(a^2\varrho)|} \left(1 + \text{const.} \, \frac{\ln|\ln(a^2\varrho)|}{|\ln(a^2\varrho)|}\right). \tag{86}$$

The other terms in the upper bound can be treated in the same way. It turns out that, choosing α large enough, all the other error terms besides the one in (86) are of lower order in $a^2 \varrho$. We omit the details. This results in the upper bound stated in Theorem 2.

APPENDIX A: PROOF OF LEMMAS 4 AND 7

We start with the three-dimensional case, Lemma 4. It suffices to show that the operator inequality (49) holds for the expectation value with any smooth function $\psi(x)$ of compact support. Given such a $\psi(x)$, define the function $\xi(x)$ by its Fourier transform $\hat{\xi}(p) = \chi(p)\hat{\psi}(p)$. We thus have to show that

$$\int_{|x| \le R} \left[|\nabla \xi(x)|^2 + \frac{1}{2} v(x) |\psi(x)|^2 \right] d^3x \ge \int_{\mathbb{R}^3} \left[(1 - \varepsilon) a U(x) |\psi(x)|^2 - \frac{a}{\varepsilon} w_R(x) |\psi(x)|^2 \right] d^3x. \tag{A1}$$

Let $\varphi(x)$ denote the solution to the zero-energy scattering equation (5), subject to the boundary condition $\lim_{|x|\to\infty}\varphi(x)=1$. Let ν be a complex-valued function on the unit sphere \mathbb{S}^2 , with $\int_{\mathbb{S}^2}|\nu|^2=1$. We use the same symbol for the function on \mathbb{R}^3 taking values $\nu(x/|x|)$. For $\psi(x)$ as above, consider the expression

$$A \equiv \int_{|x| \le R} \nu(x) \nabla \xi^*(x) \cdot \nabla \varphi(x) d^3x + \frac{1}{2} \int v(x) \psi(x)^* \varphi(x) \nu(x) d^3x.$$

We note that the last integral makes sense even in the case when v(x) has a hard core; in this case, $\frac{1}{2}v(x)\varphi(x)$ has to be interpreted as the (non-negative) measure $\Delta\varphi(x)$ (see Eq. (5)). By using the Cauchy-Schwarz inequality, we can obtain the upper bound

$$|A|^2 \leq \left(\int_{|x| \leq R} \left[|\nabla \xi(x)|^2 + \frac{1}{2} v(x) |\psi(x)|^2 \right] d^3x \right) \left(\int_{|x| \leq R} \left[|\nabla \varphi(x)|^2 + \frac{1}{2} v(x) |\varphi(x)|^2 \right] \nu(x)^2 d^3x \right).$$

Since $\varphi(x)$ is a radial function, the angular integration in the last term can be performed by using $\int_{\mathbb{S}^2} |\nu|^2 = 1$. The remaining expression is then bounded by a because of $\int_{\mathbb{R}^3} \left(|\nabla \varphi(x)|^2 + \frac{1}{2} v(x) |\varphi(x)|^2 \right) d^3x = 4\pi a$, as pointed out in the beginning of Section IV. Hence we arrive at

$$\int_{|x| \le R} \left[|\nabla \xi(x)|^2 + \frac{1}{2} v(x) |\psi(x)|^2 \right] d^3x \ge \frac{|A|^2}{a},\tag{A2}$$

for any choice of ν as above. It remains to derive a lower bound on $|A|^2$.

Note that $\varphi(x)$ is a radial function with $|\nabla \varphi(x)| = a/R^2$ for |x| = R. Hence we obtain, by partial integration,

$$\int_{|x| \le R} \nu(x) \nabla \xi^*(x) \cdot \nabla \varphi(x) d^3x = -\int_{|x| \le R} \xi^*(x) \nu(x) \Delta \varphi(x) d^3x + \frac{a}{R^2} \int_{|x| = R} \xi^*(x) \nu(x) d\omega_R,$$

where $d\omega_R$ denotes the surface measure of the ball of radius R, and we used the fact that $\nabla \nu(x) \cdot \nabla \varphi(x) = 0$. Now, by definition of h(x), $\xi(x) = \psi(x) - (2\pi)^{-3/2}h * \psi(x)$, where * denotes convolution, i.e., $h * \psi(x) = \int h(x-y)\psi(y) d^3y$. Using the zero-energy scattering equation (5) for $\varphi(x)$, we thus see that

$$A = \frac{a}{R^2} \int_{|x|=R} \psi^*(x)\nu(x) d\omega_R - (2\pi)^{-3/2} \frac{a}{R^2} \int_{|x|=R} (h * \psi)^*(x)\nu(x) d\omega_R + (2\pi)^{-3/2} \int_{|x| \le R} (h * \psi)^*(x)\nu(x) \Delta\varphi(x) d^3x.$$
(A3)

The last two terms on the right side of (A3) can be written as (note that h is a real-valued function)

$$(2\pi)^{-3/2} \int \psi^*(x) \left[\int h(y-x) \, d\mu(y) \right] \, d^3x, \tag{A4}$$

where $d\mu$ is a (non-positive) measure supported in the ball of radius R. Explicitly, $d\mu(y) = -aR^{-2}\nu(y)\delta(|y|-R)d^3y + \nu(y)\Delta\varphi(y)d^3y$. Note that $\int d\mu(y) = 0$, and also $\int d|\mu(y)| = 2a\int_{\mathbb{S}^2} |\nu| \le 2a\sqrt{4\pi}$ (by Schwarz's inequality). Hence

$$\left| \int h(y-x) \, d\mu(y) \right| \le 2a\sqrt{4\pi} f_R(x),$$

with $f_R(x)$ defined in (47). The expression (A4) is thus bounded from below by

$$(A4) \ge -(2\pi)^{-3/2} 2a\sqrt{4\pi} \int |\psi(x)| f_R(x) \, d^3x \ge -a \left(\int |\psi(x)|^2 w_R(x) \, d^3x \right)^{1/2},\tag{A5}$$

where we used Schwarz's inequality as well as the definition of $w_R(x)$ (48) in the last step. Note that this last expression is independent of $\nu(x)$.

The only place where $\nu(x)$ still enters is the first term on the right side of (A3). By choosing $\nu(x)$ to be the restriction of $\psi(x)$ to the sphere of radius R, appropriately normalized, we obtain from (A3)–(A5)

$$A \ge \frac{a}{R} \left(\int_{|x|=R} |\psi(x)|^2 d\omega_R \right)^{1/2} - a \left(\int |\psi(x)|^2 w_R(x) d^3x \right)^{1/2}.$$

Using again the Cauchy-Schwarz inequality, we see that, for any $\varepsilon > 0$,

$$|A|^{2} \ge \frac{a^{2}}{R^{2}} (1 - \varepsilon) \int_{|x| = R} |\psi(x)|^{2} d\omega_{R} - \frac{a^{2}}{\varepsilon} \int |\psi(x)|^{2} w_{R}(x) d^{3}x.$$
(A6)

In combination with (A2) this proves the desired result (A1) in the special case when U(x) is a radial δ -function sitting at a radius R, i.e., $U(x) = R^{-2}\delta(|x| - R)$. The case of a general potential U(x) follows simply by integrating this result (i.e., Ineq. (A1) for this special U(x)) against $u(R)R^2dR$, with u(R) = U(x) for |x| = R, noting that $\int u(R)R^2dR = 1$ and that $w_R(x)$ is pointwise monotone increasing in R.

The proof in the two-dimensional case, Lemma 7, follows exactly the same lines. Note, however, that the solution to the zero-energy scattering equation can not be normalized by $\lim_{|x|\to\infty} \varphi(x) = 1$ in 2D, but we can normalize it such that $\varphi(x) = 1$ for |x| = R. It then follows that $\varphi(x) = \ln(|x|/a)/\ln(R/a)$ for $R_0 \le |x| \le R$, and also that $\int_{|x|\le R} (|\nabla \varphi(x)|^2 + \frac{1}{2}v(x)|\varphi(x)|^2) d^2x = 2\pi/\ln(R/a)$ and $\int \Delta \varphi(x) d^2x = 2\pi/\ln(R/a)$ (see the appendix in [9]). The rest of the proof is unchanged, with the result that

$$\int_{|x| \le R} \left[|\nabla \xi(x)|^2 + \frac{1}{2} v(x) |\psi(x)|^2 \right] d^2x \ge \frac{1}{\ln(R/a)} \left[(1 - \varepsilon) \frac{1}{R} \int_{|x| = R} |\psi(x)|^2 d\omega_R - \frac{1}{\varepsilon} \int |\psi(x)|^2 w_R(x) d^2x \right]$$
(A7)

instead of (A2) and (A6). Multiplying this inequality with $u(R)R\ln(R/a)$, where u(R) = U(x) for |x| = R, and integrating over R using (75), we arrive at the desired result.

ACKNOWLEDGMENTS

The authors are grateful to Jakob Yngvason for several helpful discussions and remarks. The work was supported in part by the NSF grants PHY 0139984-A01 (EHL), PHY 0353181 (RS) and DMS-0111298 (JPS); by an A. P. Sloan

Fellowship (RS); by EU grant HPRN-CT-2002-00277 (JPS), by MaPhySto – A Network in Mathematical Physics and Stochastics funded by The Danish National Research Foundation (JPS), and by grants from the Danish research council (JPS).

- K. Huang, C.N. Yang, Quantum-Mechanical Many-Body Problem with Hard-Sphere Interaction, Phys. Rev. 105, 767-775 (1957).
- [2] T.D. Lee, C.N. Yang, Many-Body Problem in Quantum Mechanics and Quantum Statistical Mechanics, Phys. Rev. 105, 1119-1120 (1957).
- [3] A.L. Fetter, J.D. Walecka, Quantum Theory of Many-Particle Systems, McGraw-Hill, New York (1971).
- [4] W. Lenz, Die Wellenfunktion und Geschwindigkeitsverteilung des entarteten Gases, Z. Phys. 56, 778–789 (1929).
- [5] E.H. Lieb, J. Yngvason, Ground State Energy of the Low Density Bose Gas, Phys. Rev. Lett. 80, 2504–2507 (1998).
- [6] F.J. Dyson, Ground-State Energy of a Hard-Sphere Gas, Phys. Rev. 106, 20–26 (1957).
- [7] M. Schick, Two-dimensional System of Hard Core Bosons, Phys. Rev. A 3, 1067–1073 (1971).
- [8] D. F. Hines, N. E. Frankel, D. J. Mitchell, Hard disc Bose gas, Phys. Lett. 68A, 12–14 (1978).
- [9] E.H. Lieb, J. Yngvason, The Ground State Energy of a Dilute Two-Dimensional Bose Gas, J. Stat. Phys. 103, 509–526 (2001).
- [10] G.A. Baker, Singularity Structure of the Perturbation Series for the Ground-State Energy of a Many-Fermion System, Rev. Mod. Phys. 43, 479–531 (1971).
- [11] H.-W. Hammer, R.J. Furnstahl, Effective field theory for dilute Fermi systems, Nucl. Phys. A 678, 277–294 (2000).
- [12] R. Seiringer, The Thermodynamic Pressure of a Dilute Fermi Gas, in preparation.
- [13] D. Ruelle, Statistical Mechanics. Rigorous Results, World Scientific (1999).
- [14] D.W. Robinson, The Thermodynamic Pressure in Quantum Statistical Mechanics, Springer Lecture Notes in Physics, Vol. 9 (1971).
- [15] E. H. Lieb, M. Loss, Analysis, Amer. Math. Soc. (2001).
- [16] G.M. Graf, J.P. Solovej, A correlation estimate with applications to quantum systems with Coulomb interactions, Rev. Math. Phys. 6, 977–997 (1994).
- [17] E.H. Lieb, H.-T. Yau, The Stability and Instability of Relativistic Matter, Commun. Math. Phys. 118, 177–213 (1988).
- [18] P. Li, S.-T. Yau, On the Schrödinger equation and the eigenvalue problem, Commun. Math. Phys. 88, 309–318 (1983).